Supporting Information

Improved Ductility of B_{12} Icosahedra-based Superhard Materials through Icosahedral Slip

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Table S1. The predicted bulk modulus, shear modulus, hardness and ideal shear stress for $(o\text{-}B_{10}Si_2)Si_2$, $(m\text{-}B_{10}Si_2)Si_2$ and $(B_{11}C_p)CBC$. The predicted elastic moduli for $(o\text{-}B_{10}Si_2)Si_2$ and $(m\text{-}B_{10}Si_2)Si_2$ are listed in Table S2 and S3,respectively.

Structure	$(o\text{-}B_{10}Si_2)Si_2$	$(m\text{-}B_{10}Si_2)Si_2$	$(B_{11}C_p)CBC$
Bulk modulus (GPa)	160.1	159.7	238.0
Shear modulus (GPa)	136.6	138.3	199.0
Theoretical Vickers hardness (GPa)	26.5	27.2	32.9
Theoretical Knoop hardness (GPa)	23.5	27.7	34.3
Ideal shear stress (GPa)	26.3	27.5	39.0

Table S2. The predicted elastic constant (unit: GPa) for (o-$B_{10}Si_2$)Si_2

C_{ij}	XX	YY	ZZ	XY	YZ	ZX
XX	360.16	78.54	63.67	-4.46	-8.93	-7.13
YY	78.54	363.56	63.48	0.32	-1.86	-8.77
ZZ	63.67	63.48	312.05	0.23	-0.95	-1.47
XY	-4.46	0.32	0.23	136.43	-0.68	-3.45
YZ	-8.93	-1.86	-0.95	-0.68	135.94	-0.97
ZX	-7.13	-8.77	-1.47	-3.45	-0.97	135.22

Table S3. The predicted elastic constant (unit: GPa) for (m-$B_{10}Si_2$)Si_2

C_{ij}	XX	YY	ZZ	XY	YZ	ZX
XX	351.92	69.02	74.17	-7.52	10.24	5.54
YY	69.02	332.18	70.02	-9.50	12.82	7.85
ZZ	74.17	70.02	334.03	-3.46	10.59	5.95
XY	-7.52	-9.50	-3.46	135.39	2.72	1.29
YZ	10.24	12.82	10.59	2.72	142.55	-3.75
ZX	5.54	7.85	5.95	1.29	-3.75	146.80

Figure S1.

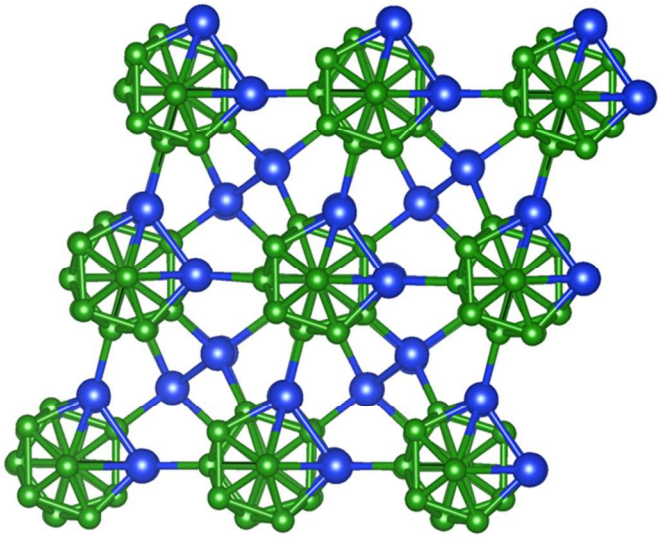
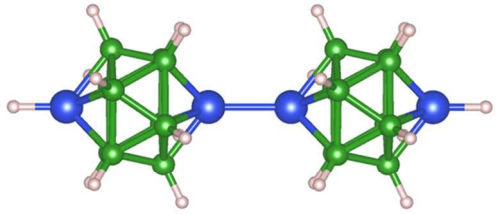
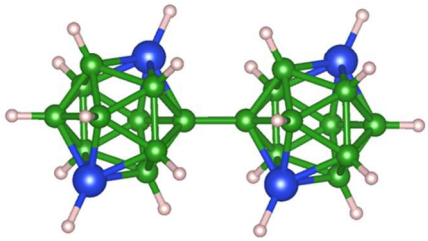


Figure S1. Final snapshot of (o-$B_{10}Si_2$)Si_2 in *ab initio* molecular dynamics (AIMD) simulations at 300 K. No ($B_{10}Si_2$) icosahedra deconstruct in dynamics, indicating that this structure is stable at finite temperature.

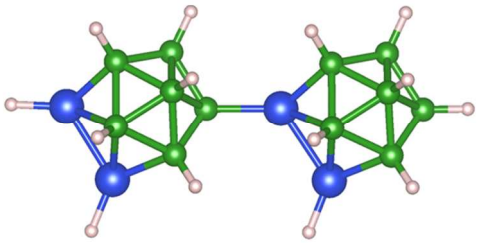
Figure S2



(a) $(B_{10}SiH_{11})Si\text{-}Si(B_{10}SiH_{11})$



(b) $(B_9Si_2H_{11})B\text{-}B(B_9Si_2H_{11})$



(c) $(B_{10}SiH_{11})Si\text{-}B(B_9Si_2H_{11})$

Figure S2. Finite icosahedral clusters to represent the inter-icosahedral bonds in $(p\text{-}B_{10}Si_2)Si_2$ and $(o\text{-}B_{10}Si_2)Si_2$: (a) Si-Si bond in $(p\text{-}B_{10}Si_2)H_{12}$; (b) B-B bond in $(p\text{-}B_{10}Si_2)H_{12}$; and (c) Si-B bond in $(o\text{-}B_{10}Si_2)H_{12}$.

Figure S3

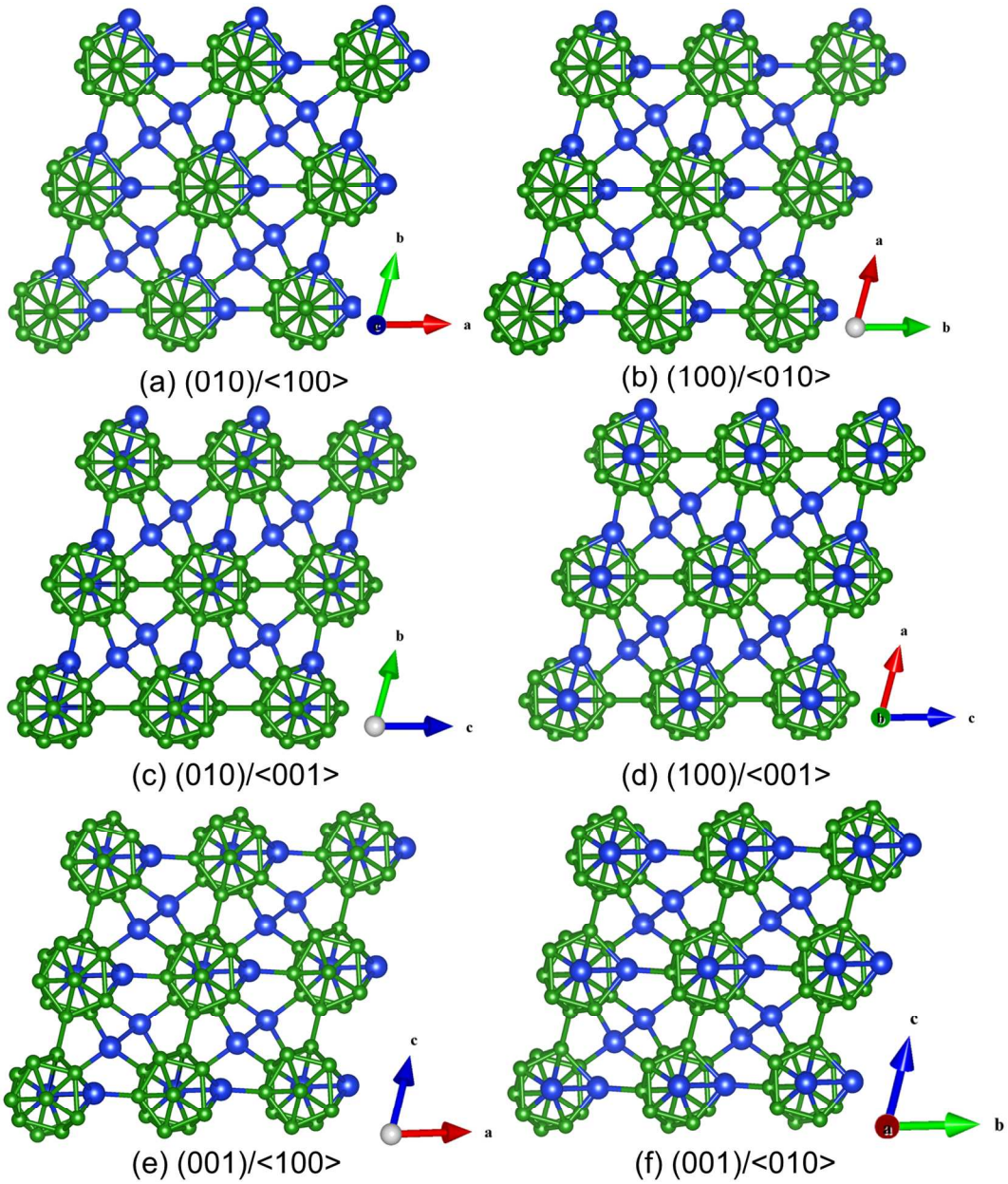


Figure S3. Plausible slip systems for (o-$B_{10}Si_2$)Si_2 belonging to {001}/[100] slip system. Shearing along slip systems (010)/<100> (a) and (100)/<010> (b) are the same because of the symmetry of the crystal. They are also the same for the (010)/<001> (c) and the (100)/<001> (d), and for the (001)/<100> (e) and the (001)/<010> (f).

Figure S4

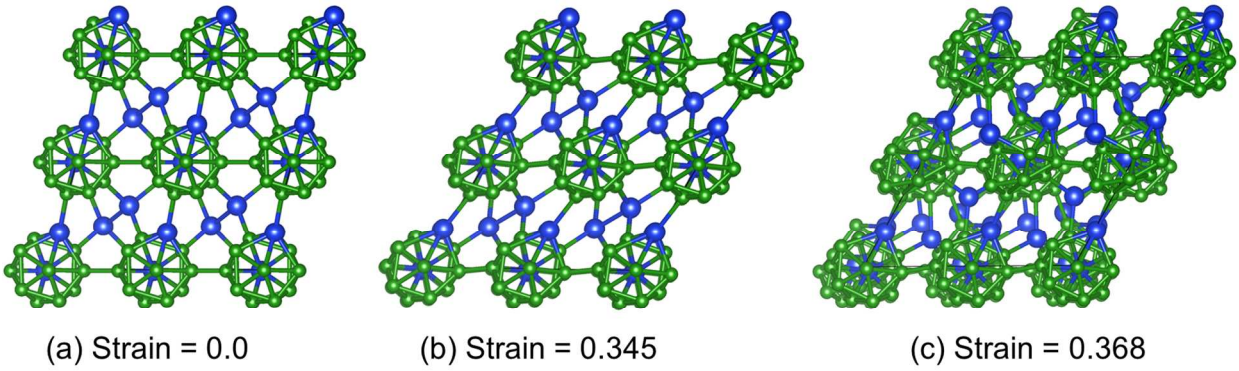


Figure S4. The structural changes for (m-$B_{10}Si_2$)Si_2 shearing along (100)/<001> slip system: (a) intact structure; (b) structure at 0.345 strain before the failure; (c) structure at 0.368 strain after stress release where the ($B_{10}Si_2$) icosahedra are disintegrated.